# Integrability-based analysis of the hyperfine interaction induced decoherence in quantum dots

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Using the Algebraic Bethe Ansatz (ABA) in conjunction with a simple Monte Carlo (MC) sampling technique, we study the problem of the decoherence of a central spin coupled to a nuclear spin bath. We describe in detail the full crossover from strong to weak external magnetic field field, a limit where a large non-decaying coherence factor is found. This feature is explained by Bose-Einstein-condensate (BEC)-like physics which also allows us to argue that the corresponding zero frequency peak would not be broadened by statistical or ensemble averaging.



Using the spin of a single electron (or hole) trapped in semiconductor-based quantum dots has been a long standing proposal for a possible implementation of a qubit [1] for which single-spin readout and coherent control [2] is now possible. In these setups, the isotropic Fermi contact hyperfine interaction of the trapped central spin with the bath of nuclear spins present in the substrate is know to be the essential source of decoherence leading, over time, to a loss of the information encoded in any prepared state of the central spin. Denoting by $\vec{S}_0$ the central spin-$\frac{1}{2}$, by $\vec{I}_j$ the $N$ nuclear spins, and by $g$ and $g_n$ the respective couplings to the external magnetic field $h$, the Hamiltonian reads

$$H = ghS_0^z + g_{\rm n}h\sum_{j=1}^{N} I_j^z + \sum_{j=1}^{N} A_j \vec{S}_0 \cdot \vec{I}_j. \qquad (1)$$

Dropping an irrelevant constant the first two terms can be simplified [3, 4] to $BS_0^z$ with $B = (g - g_{\rm n})h$.

In the regime of strong magnetic field $B > A$, with $A$ being $N$ times the largest $A_j$, the time evolution of the central spin $\langle \vec{S}_0(t)\rangle$ can be described perturbatively [3, 5–8] in the flip-flop terms $\sum_j A_j(S_0^+ I_j^- + \text{h.c.})$. In a detailed study to fourth order Coish *et al.* [7] found that the Larmor precession undergoes a typical exponential decay which is supplemented by additional low-frequency envelope modulations. In the opposite limit of weak (or intermediate) fields a variety of methods including semiclassics, exact diagonalization, or the ABA have been applied [5, 8–12]. For unpolarized spin baths at $B = 0$, extrapolating a semi-classical approach [9] to the continuum limit, as well as time-dependent mean field theory [11] for very large systems with $N = 16000$ showed logarithmic decay $\langle S_0^z(t)\rangle \sim 1/\ln(t)$ at long times. However, all approaches in the weak field limit are either based on mean-field/semi-classics or are restricted to either very small system sizes $N \leq 20$, specific bath polarizations, or the short-time behavior.

In this work we aim to overcome these limitations by developing a hybrid method based on the ABA in combination with a direct MC sampling of the exact eigenstates of the system, which we apply to the transverse relaxation of the central spin. The method provides a non-perturbative full quantum treatment giving us access to the complete crossover from strong to weak field without any restriction on the initial polarization of the bath. Due to the trivial time evolution in the eigenbasis, it also provides access to real-time dynamics at arbitrarily long times without accumulated errors. While it is only usable for modest system sizes, recent developments have drastically sped up the computation time. In this work we treat systems containing up to $N = 48$ nuclear spins whose Hilbert space is $\sim 2 \times 10^8$ times larger than the ones previously treated with exact methods [8, 10].

For the dynamics of $\langle S^+(t)\rangle$ we find the following conclusions: (i) At strong to intermediate fields we observe exponential decay with weak modulations and thus confirm the perturbative picture [7]. (ii) For smaller fields, these weak modulation become dominant leading to long-lived slow oscillations. (iii) As $B \to 0$, an initial rapid decay is followed by the formation of a non-decaying coherent fraction whose amplitude and phase is in one-to-one correspondence with the initial state of the central spin. This lack of decay is explained as a consequence of BEC-like physics. (iv) We argue that the non-decaying fraction survives ensemble averaging and is at most logarithmically dependent on finite size effects. Consequently, we expect it to be experimentally observable.

To be specific, we will consider nuclear spins $\frac{1}{2}$ although this restriction is not imposed by integrability or the numerical method. The couplings are chosen as $A_j = \frac{A}{N}e^{-(j-1)/N}$ corresponding to a Gaussian electronic wavefunction in a 2D quantum dot [3]. We study in detail the time-evolution of an initial coherent superposition of the central spin: $\frac{1}{\sqrt{2}}(|\Uparrow\rangle + |\Downarrow\rangle)$ related to the $T_2$ transverse relaxation time. We assume the initial condition to be a product state $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|\Uparrow\rangle + |\Downarrow\rangle) \otimes |\Psi_{\rm bath}\rangle$, with $|\Psi_{\rm bath}\rangle$ describing the nuclear spins. Narrowing techniques [13] will typically allow one to create a superposition of (nearly-)degenerate eigenstates of the Overhauser operator $h^z = \sum_{j=1}^{N} A_j I_j^z$. Provided there is no special phase relation between them, the density matrix can be reduced to its diagonal terms, leading to an averaged sum

over the represented $h^z$ eigenstates. Here we avoid the average by using a single specific zero-polarization "maximal entropy" state: $|\Psi_{\rm bath}\rangle = |\downarrow_1\uparrow_2\downarrow_3\uparrow_4\cdots\rangle$ with the eigenvalue $h^z_{\rm init} = \sum_{j=1}^N (-1)^j A_j/2$. Having the up-pointing spins uniformly spread out over the full range of available coupling strengths should make this state sufficiently generic to capture the dominant features of a diagonal ensemble average. We will confirm the validity of this particular choice by explicitly comparing randomly generated initial nuclear configurations.

Our main quantity of interest is the central spin coherence factor which, projecting on the eigenbasis of $H$, can be written as

$$\langle S_0^+(t)\rangle = \langle\Psi(t)|\, S_0^+\,|\Psi(t)\rangle = \sum_{m,n} C_{m,n} e^{i(\omega_m-\omega_n)t}, \quad (2)$$

where $C_{m,n} = \langle\Uparrow;\Psi_{\rm bath}\,|\psi_m\rangle\,\langle\psi_m|\,S_0^+\,|\psi_n\rangle\,\langle\psi_n\,|\Downarrow;\Psi_{\rm bath}\rangle$ with $|\psi_m\rangle$ and $|\psi_n\rangle$ denoting eigenstates of the Hamiltonian (1) with energies $\omega_m$ and $\omega_n$ respectively. Since $S_0^z + \sum_{j=1}^N I_j^z$ is conserved, $|\psi_m\rangle$ must contain one more up-spin than $|\psi_n\rangle$.

Any eigenstate of the central spin model (1) is entirely defined by $M$ complex rapidities $\{\lambda_1 ... \lambda_M\}$ which are a solution of the system of $M$ coupled non-linear algebraic Bethe equations

$$-2B + \sum_{k=0}^{N} \frac{1}{\lambda_i - \epsilon_k} - \sum_{j=1(\neq i)}^{M} \frac{2}{\lambda_i - \lambda_j} = 0. \quad (3)$$

Here $\epsilon_k = -1/A_k$ and $\epsilon_0 = 0$. For every solution of (3) the corresponding (unnormalized) eigenstate is obtained by the repeated action, for each rapidity, of a generalized creation operator $\mathrm{S}^+(\lambda_i) \equiv \sum_{k=0}^N \frac{S_k^+}{\lambda_i-\epsilon_k}$, i.e. $|\{\lambda_1 ... \lambda_M\}\rangle = \prod_{i=1}^M \mathrm{S}^+(\lambda_i)\,|\Downarrow;\downarrow\downarrow ... \downarrow\rangle$. The corresponding eigenenergy is then given by

$$E(\{\lambda_1 ... \lambda_M\}) = \frac{1}{2}\sum_{i=1}^{M}\frac{1}{\lambda_i} - \frac{B}{2} - \frac{1}{4}\sum_{j=1}^{N}\frac{1}{\epsilon_j}. \quad (4)$$

Due to the level of difficulty of systematically finding solutions to Eq. (3) we solve instead for a different set of variables $\Lambda(\epsilon_i) = \sum_{j=1}^M \frac{1}{\epsilon_i - \lambda_j}$, which can be shown to obey a simpler set of quadratic equations [14, 15]. Any given solution to these equations is found starting from the trivial $B = \infty$ solutions where an ensemble of $M$ spins are pointing up and the remaining $N-M$ are pointing down. These configurations are deformed by a stepwise ramping of the $1/B$-parameter until the desired $B$ value is reached [15] . Finally, it was recently shown that the scalar products matrix elements defining $C_{m,n}$ in Eq. (2) can be written, in terms of $\Lambda(\epsilon_i)$, as determinants of $N+1$ by $N+1$ matrices [16]. The resulting fast algorithm allows us to define a probability $P_{m,n} \equiv |C_{m,n}|$ for any pair of eigenstates $(m,n)$ and perform the double sum in Eq. (2) using a simple Metropolis algorithm (see [17] for another example of combining MC with ABA). Starting from a randomly selected pair of $B=\infty$ eigenstates, we first deform them to the desired finite-$B$ eigenstates $|\psi_m\rangle, |\psi_n\rangle$ and compute the probability $P_{m,n}$, frequencies $\omega_m, \omega_n$ and the sign $s_{m,n} = \mathrm{sgn}(C_{m,n})$. A new pair is then generated by randomly selecting one of the two $B=\infty$ configurations and minimally changing it by exchanging a randomly selected pair of up and down spin. Deforming this new configuration to finite $B$ we compute $P_{m,n'}$ (assuming state $n$ was modified) and accept the new pair $(m,n')$ with probability $\max\left(1, \frac{P_{m,n'}}{P_{m,n}}\right)$. Repeating the procedure generates a list of $\Omega$ configurations $(m_\alpha, n_\alpha)$ distributed according to $P_{m_\alpha,n_\alpha}$ such that

$$\frac{< S_0^+(t) >}{< S_0^+(0) >} = \lim_{\Omega\to\infty} \frac{\sum_{\alpha=1}^{\Omega} s_{m_\alpha,n_\alpha} e^{i(\omega_{m_\alpha}-\omega_{n_\alpha})t}}{\sum_{\alpha=1}^{\Omega} s_{m_\alpha,n_\alpha}}, \quad (5)$$

which can be normalized by the known initial value of the coherence factor. Figure 1 presents the spectrum $\langle S_0^+\rangle(\omega)$ and its Fourier transform $\langle S_0^+(t)\rangle$ for a wide range of external magnetic fields covering the full non-perturbative crossover $B_{\rm fluc} \lesssim B \lesssim A$, where $B_{\rm fluc} = (\sum_{j=1}^N A_j^2)^{1/2}$ is a typical Overhauser field due to spin fluctuations [18], all the way down to very weak magnetic fields. All plots are obtained for an ensemble of $N = 36$ nuclear spins by sampling $\Omega = 10^7$ configurations. For any finite size system, the spectrums consist of a series of delta peaks which are smoothed into Lorentzians of width $0.001B$ in the plots. We stress that this broadening is much smaller than the width of the peaks seen on the graphs, i.e. the peaks are composed of a large number of contributions at similar frequencies.

The spectrum is basically characterized by two structures. First we find a peak around the "bare" Larmor frequency $B + h^z_{\rm init}$ given by the total effective magnetic field felt by the central spin. For the strongest magnetic fields this sharp peak is the dominant feature whose nearly Lorentzian lineshape leads to exponentially decaying oscillations. As the magnetic field is lowered its width increases giving rise to faster decoherence. In addition, there is a low-frequency structure which carries a very low weight at strong fields but leads to slow modulations of the envelope function. These modulations were previously observed in the fourth order perturbative treatment [7] and are now confirmed by our exact results.

When lowering the field below $B_{\rm fluc} \approx 0.1\,A$ the low-frequency structure becomes the dominant feature, eventually taking a scaling form of $\omega/B$ for sufficiently weak fields (see Fig. 1.c). The low-frequency structure has a finite width ($\propto B$) and, as $B \to 0$, collapses into a delta peak. In the long-time dynamics, this leads to the slowly decaying low-frequency oscillations shown in Fig. 1.e), whose period and lifetime can be made arbitrarily large since the real-time evolution becomes a function of $Bt$. As $B \to 0$ this ultimately gives rise to a non-decaying fraction representing nearly 0.5 of the initial value. At

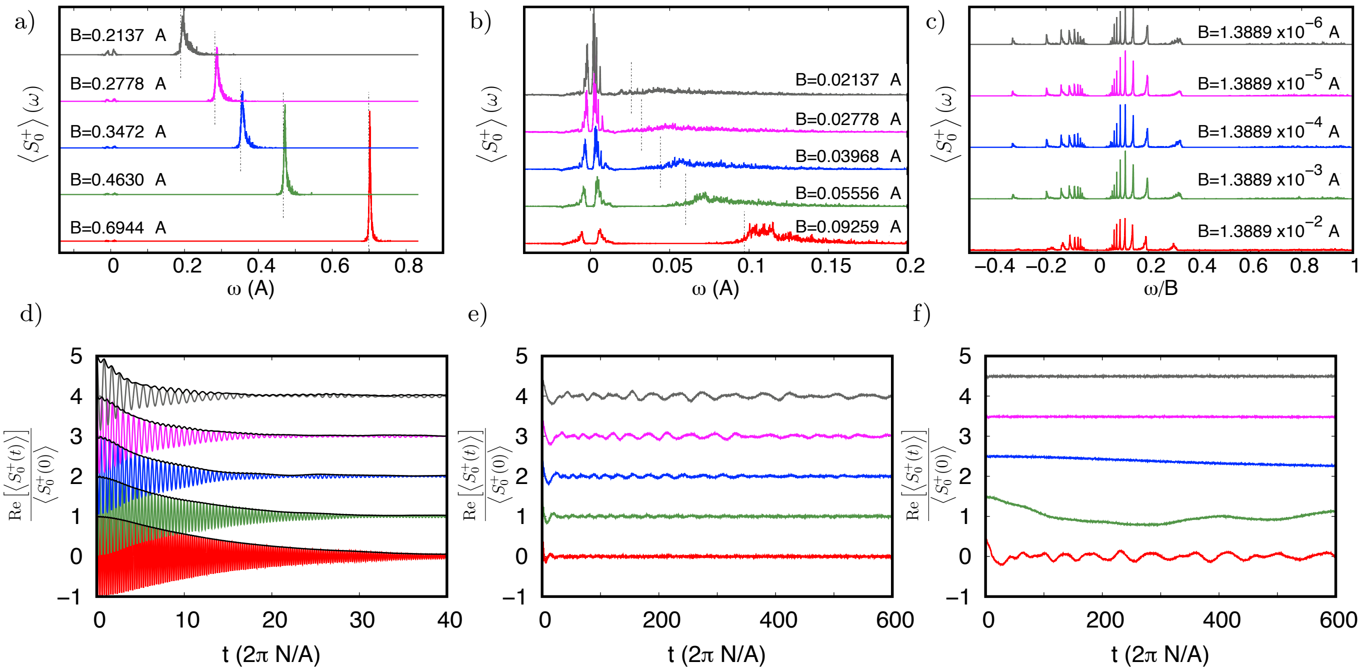


FIG. 1. Top: Spectrum $\langle S_0^+(\omega)\rangle$ in the crossover and weak magnetic field regimes. The dashed lines mark the "bare" Larmor frequencies $B + h^z_{\mathrm{init}}$. Panel c) is plotted in terms of the rescaled frequency $\omega/B$ and shows only the low-frequency structure. Bottom: The corresponding real-time evolution of the coherence factor $\langle S_0^+(t)\rangle$. Each curve has an offset of 1 compared to the previous one. Black lines in panel d) are the norms $\left|\langle S_0^+(t)\rangle\right|$ which, in the perturbative regime, correspond to the envelope function computed in [7].

$B = 0$ the total coherence factor $\langle S_0^+\rangle + \sum_{j=1}^N \langle I_j^+\rangle$ is conserved, hence the lost central spin coherence is transferred to the nuclear spins polarizing them along the central spin's initial orientation and ultimately locking the system into a non-decaying steady state.

Here, by working with exact eigenstates of the model we get valuable insight in the processes involved which allow us to demonstrate the complete absence of long-time decay, i.e. in contrast to other approaches [9, 11] we do not observe a $1/\ln(t)$ decay. Indeed, we know that in the $B \to 0$ limit, solutions to the Bethe equations (3) split into two independent subsets. A state-dependent number $0 \le r \le M$ of rapidities diverge as $\lambda_i \approx L_i/B + \mathcal{O}(1)$ ($L_i$ being roots of a Laguerre polynomial [19]). For these, the creation operator $\mathrm{S}^+(\lambda_i \to \infty) \propto \sum_{k=0}^N S_k^+$ creates fully delocalized excitations whose contribution to the energy is $1/\lambda_i \propto B + \mathcal{O}(B^2)$. The remaining $M - r$ rapidities stay finite $\lambda_i \approx \lambda_i^0 + \mathcal{O}(B)$ and create localized excitations (due to the proximity of $\lambda_i$ with some particular values of the inverse couplings $\{\epsilon_i\}$). They contribute a finite energy $1/\lambda_i \propto \text{const.} + \mathcal{O}(B)$. These two subsets being decoupled, any set of $r_f$ finite rapidities solution to the $B = 0$ Bethe equations (3) can be supplemented by any number $r < N - r_f$ of diverging rapidities to create exact $B = 0$ eigenstates containing $r + r_f$ rapidities, $\left[\mathrm{S}^+(\infty)\right]^r \left[\prod_{i=1}^{r_f} \mathrm{S}^+(\lambda_i^0)\right] |\Downarrow; \downarrow\downarrow \dots \downarrow\rangle$, which all have the same energy. This can be thought of as a manifestation of BEC-like physics since it allows one to build eigenstates by adding any number of particles in a given single quantum state. It echoes the behavior of other integrable Gaudin models such as Dicke model's superradiance [20] or Richardson model's superconductivity [21].

Thus for any $M$-particle eigenstate $|\psi_n\rangle$, there exists a corresponding $M+1$ eigenstate which, at $B = 0$, only differs by adding a single delocalized zero-energy particle. Any such pair of eigenstates leads, in Eq. (2), to a low-frequency contribution at $\omega = \omega_m - \omega_n \propto B$ and contributes to the non-decaying fraction at $B = 0$. Any other pair of eigenstates gives a contribution at a finite frequency which, being spread over a large energy band, leads to an initial rapid decay. Since the energies are only related to the finite rapidities content of the states, weak magnetic fields will only give subleading corrections. As shown in Fig. 2 for $B \lesssim B_{\mathrm{fluc}}$, this results in a saturation of the decay time characterizing the early dynamics which become well captured by a quadratic decay independent of the magnetic field value.

Experimental observation of the non-perturbative long-time contributions, e.g. the low-frequency oscillations, requires two conditions. It needs to have a lifetime sufficiently longer than the initial decay and, at the same time, it has to carry a sufficiently large weight. From a rough analysis of the real-time numerical data, fields $B \le 0.03A$ ($\sim 0.1\,\mathrm{T}$ for GaAs or $\sim 0.0015\,\mathrm{T}$ for Si:P using [3] $A/(g^*\mu_B) = 3.5\,\mathrm{T}$ and $A/(g^*\mu_B) = 0.05\,\mathrm{T}$

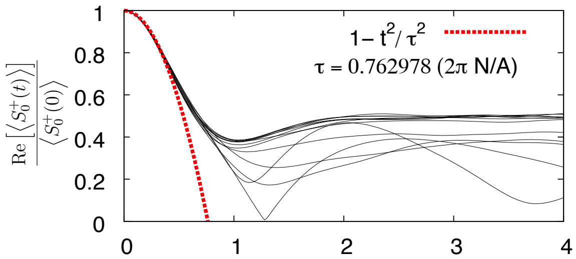


FIG. 2. Short time dynamics of the norm $\left|\left\langle S_0^+(t)\right\rangle\right|$ for intermediate to weak fields. The nine values of magnetic fields $B < B_{\text{fluc}}$ shown in Fig. 1 are plotted with black lines ($B/A \in \left[1.3889 \cdot 10^{-6}, 0.05556\right]$). The red line is a quadratic fit with parameter $\tau \sim (A/N)^{-1}$. For both GaAs and Si:P, using values from [3] gives $\tau \approx 1\mu$s.

respectively) would be sufficient to exhibit oscillations with an amplitude of $\sim 10\%$ of the initial coherence factor and a lifetime long enough compared to the initial rapid decay (see the $B = 0.02778(A)$ curve in Fig. 1.e). These oscillations would be clearly distinguishable from any perturbative result since their frequency is nearly an order of magnitude lower than the Larmor frequency. Since we are looking for a clear measurable signature, the resulting threshold is at much weaker fields than the naive limit of validity of perturbation theory $B \sim A$.

In Fig. 3 we show the long-time averaged contribution for a variety of system sizes. We see that even for modest system sizes ($N \geq 20$) the finite-size discretization does not seem to affect strongly the total weight carried by the low-frequency contributions. The error bars and system sizes treated here do not exclude a slow logarithmic reduction $\sim 1/\ln(\beta N)$ of the total fraction as was observed in a finite-size semi-classical treatment [9] of the longitudinal decay, eventually leading to $1/\ln(t)$ decay in the continuum limit [9]. In contrast, our full quantum mechanical treatment includes the discreteness of the spin bath and shows the non-decaying fraction to be a observable for finite systems. Indeed, even an as-

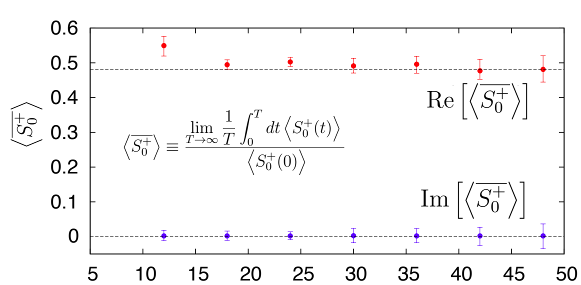


FIG. 3. Non-decaying coherent fraction as a function of the number of nuclear spins at $B/A = 1.04168 \cdot 10^{-6}$. We sample $\Omega = 10^7$ configurations. Error bars indicate the magnitude of the fluctuations which are due to a mixture of finite size effects and MC error. Dashed lines are guides to the eye at 0 and 0.4812 (long-time values for $N = 48$).

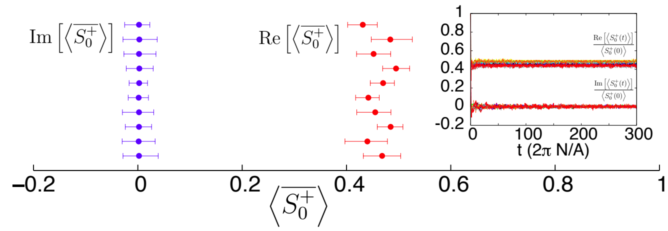


FIG. 4. Long-time averaged coherent fraction for 10 randomly generated initial nuclear spin configurations. The meaning of the error bars is as in Fig. 3. Inset: Corresponding real-time evolution. Magnetic field is $B/A = 1.3889 \times 10^{-6}$.

sumed $\sim 1/\ln(\beta N)$ reduction would yield an observable non-decaying fraction for experimentally relevant system sizes ($N \approx 10^2$ in Si:P or $N \approx 10^5$ in GaAs).

Considering that even a physically narrowed system should be described in terms of a diagonal ensemble average, in Fig. 4 we compare the weak field dynamics for an ensemble of 10 unpolarized ($M = N/2$) initial bath states obtained by choosing a random set of $M$ up-pointing nuclear spins. This is less restrictive than the eigenstate content of a narrowed state since the initial Overhauser eigenvalue $h^z_{\text{init}}$ is not fixed. While we observe slight variations in the total non-decaying fraction, it systematically stays above 0.4 and maintains the X-Y plane phase of the initial central spin orientation. Initializing the central spin at a different point on the Bloch sphere $\alpha\left|\Uparrow\right\rangle + \beta\left|\Downarrow\right\rangle$ would only lead to a multiplicative factor $\left\langle S_0^+(t)\right\rangle = \alpha\beta\left\langle S_0^+(t)\right\rangle_{(\Uparrow+\Downarrow)}$ which still conserves the relative phase. Albeit averaging may lead to a slightly lowered total fraction, the common phase obtained for all nuclear spin configurations means that diagonal ensemble averages $\left\langle S_0^+(t)\right\rangle \equiv \sum_n \gamma_n \left\langle\{\epsilon\}_n\right| S_0^+(t) \left|\{\epsilon\}_n\right\rangle$, be they performed for a narrowed or even infinite temperature state, would still yield a large non-decaying fraction.

Since it is linked to diverging rapidities, the existence of a "condensate" mode is completely independent of the set of couplings constants and hence the dot geometry. Therefore, the zero-frequency peak which leads to a non-decaying fraction, should not exhibit any inhomogeneous broadening in experiments which involve an average over different quantum dots. In fact, neither the geometry nor the initial nuclear spin configuration affect the resulting delta peak. This is in stark contrast to recent optical spin noise experiments [22] where a Lorentzian lineshape was observed. However, a direct comparison to our results is not possible considering the experimental work was carried out on hole-spin based samples for which the hyperfine coupling is strongly anisotropic.

In the isotropic system considered here a finite lifetime would require the addition of integrability breaking terms to the Hamiltonian (1). The weak dipolar coupling between the nuclear spins could play such a role although on relatively long time scales $\tau_{dd} \approx 10^{-4}$ s in GaAs; an-

other mechanism would be quadrupole couplings to the nuclear spins [23]. In addition, while we argued that ensemble fluctuations in the nuclear Overhauser field would not lead to a finite lifetime, it should be noted that local fluctuations in the external magnetic field would induce broadening due to the $\omega/B$ dependency of the spectrum. This demonstrates that, at weak field, the strong correlations between the central and nuclear spins lead to a clear distinction between external magnetic field and the internal Overhauser field.

In conclusion, we have developed a non-perturbative method to study the dynamics in the central spin model which is applicable to arbitrary magnetic fields and initial bath polarizations and provides access to the real-time dynamics at arbitrary long times. We applied this method to the transverse spin relaxation which, at weak fields, shows initial rapid quadratic decay followed by a large arbitrarily long-lived finite coherent fraction resulting from the BEC-like behavior of the system.

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